von Neumann-Landau equation for wave functions, wave-particle duality and collapses of wave functions

Zeqian Chen*

State Key Laboratory of Magnetic Resonance and Atomic and
Molecular Physics and United Laboratory of Mathematical Physics,
Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences,
30 West District, Xiao-Hong-Shan, P.O.Box 71010, Wuhan, China

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It is shown that von Neumann-Landau equation for wave functions can present a mathematical formalism of motion of quantum mechanics. The wave functions of von Neumann-Landau equation for a single particle are 'bipartite', in which the associated Schrödinger's wave functions correspond to those 'bipartite' wave functions of product forms. This formalism establishes a mathematical expression of wave-particle duality and that von Neumann's entropy is a quantitative measure of complementarity between wave-like and particle-like behaviors. Furthermore, this extension of Schrödinger's form suggests that collapses of Schrödinger's wave functions can be regarded as the simultaneous transition of the particle from many levels to one.

I.   INTRODUCTION

As is well known, Heisenberg's equation [1] and Schrödinger's equation [2], as two forms for the equations of motion of quantum mechanics, are equivalent. Of these, the Schrödinger form seems to be the more useful one for practical problems, as it provides differential equations for wave functions, while Heisenberg's equation involves as unknowns the operators forming the representative of the dynamical variable, which are far more numerous and therefore more difficult to evaluate than the Schrödinger unknowns. Also, determining energy levels of various dynamic systems is an important task in quantum mechanics, for this solving Schrödinger's wave equation is a usual way. Recently, Fan and Li [3] showed that Heisenberg's equation can also be used to deduce the energy level of some systems. By introducing the conception of invariant 'eigen-operator', they derive energy-level gap formulas for some dynamic Hamiltonians. However, their 'invariant eigen-operator' equation involves operators as unknowns, as similar to Heisenberg's equation, and hence is also difficult to evaluate in general.

On the other hand, wave-particle duality, as manifest in the two-slit experiment, provides perhaps the most vivid illustration of Bohr's complementarity principle which refers to the ability of quantum-mechanical entities to behave as waves or particles under different experiment conditions [4]. Wave-like (interference) behaviour can be explained by the superposition principle [5], while the usual explanation for the loss of interference (particle-like behaviour) in a which-way experiment is based on Heisenberg's uncertainty principle [6]. However, it is demonstrated in the which-way ex-

periment with an atom interferometer that Heisenberg's position-momentum uncertainty relation cannot explain the loss of interference for which the correlations between the which-way detector and the atomic beams are considered to be responsible [7]. From a theoretical point of view, a measurement-free express of wave-particle duality deserves research.

In this article, we show that von Neumann-Landau equation for wave functions (vNLW) is an extension of Schrödinger's wave equation and can be used to determine energy-level gaps of the system. Contrary to Schrödinger's wave equation, vNLW is on 'bipartite' wave functions. It is shown that these 'bipartite' wave functions satisfy all the basic properties of Schrödinger's wave functions which correspond to those 'bipartite' wave functions of product forms. In particular, we will show that this extension of Schrödinger's form establishes a mathematical expression of wave-particle duality and that von Neumann's entropy is a quantitative measure of complementarity between wave-like and particle-like behaviors. Furthermore, from this formalism it is concluded that collapses of Schrödinger's wave functions can be regarded as the simultaneous transition of the particle from many levels to one.

II.   VON NEUMANN-LANDAU EQUATION FOR WAVE FUNCTIONS

Consider the quantum system of a single particle. Note that the Hamiltonian for a single particle in an external field is

$$\hat{H}(\vec{x}) = -\frac{\hbar^2}{2m}\nabla_{\vec{x}}^2 + U(\vec{x}), \qquad (2.1)$$

where $\nabla_{\vec{x}}^2 = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$, $U(\vec{x})$ is the potential energy of the particle in the external field, and $\vec{x} = (x_1, x_2, x_3) \in \mathbf{R}^3$. The Schrödinger's wave equation

*Electronic address: zqchen@wipm.ac.cn

describing dynamics of the particle is

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} = \hat{H}(\vec{x})\psi(\vec{x},t) = -\frac{\hbar^2}{2m}\nabla^2_{\vec{x}}\psi(\vec{x},t)+U(\vec{x})\psi(\vec{x},t).$$
(2.2)

The state of the particle can be described by a definite wave function ψ of Equation (2.2), whose stationary states determine its energy levels. Moreover, the expectation value of an observable $\hat{Q}$ in the state corresponding to ψ is determined by $\langle\hat{Q}\rangle_\psi = \langle\psi|\hat{Q}|\psi\rangle$.

On the other hand, let $\psi(\vec{x},t)$ and $\varphi(\vec{x},t)$ both satisfy Eq.(2.2). Then we have

$$i\hbar\frac{\partial(\psi(\vec{x},t)\varphi^*(\vec{y},t))}{\partial t}$$
$$= i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t}\varphi^*(\vec{y},t) + i\hbar\frac{\partial\varphi^*(\vec{y},t)}{\partial t}\psi(\vec{x},t)$$
$$= \left[\hat{H}(\vec{x})\psi(\vec{x},t)\right]\varphi^*(\vec{y},t) - \left[\hat{H}(\vec{y})\varphi(\vec{y},t)\right]^*\psi(\vec{x},t)$$
$$= \left(\hat{H}(\vec{x}) - \hat{H}(\vec{y})\right)(\psi(\vec{x},t)\varphi^*(\vec{y},t)).$$

This leads to the following wave equation

$$i\hbar\frac{\partial\Psi(\vec{x},\vec{y};t)}{\partial t} = \left(\hat{H}(\vec{x}) - \hat{H}(\vec{y})\right)\Psi(\vec{x},\vec{y};t), \qquad (2.3)$$

where $\Psi(\vec{x},\vec{y};t) \in L^2_{\vec{x},\vec{y}}$. Contrary to Schrödinger's wave equation Eq.(2.2) for 'one-partite' wave functions $\psi(\vec{x}) \in L^2_{\vec{x}}$, the wave equation Eq.(2.3) is an differential equation for 'bipartite' wave functions $\Psi(\vec{x},\vec{y})$, which, replacing $\hat{H}(\vec{x}) + \hat{H}(\vec{y})$ by $\hat{H}(\vec{x}) - \hat{H}(\vec{y})$, is also different from Schrödinger's wave equation for two particles.

We would like to mention that Eq.(2.3) has been presented by von Neumann [8] and Landau [9] giving the change in the density matrix with time. Here, we regard Eq.(2.3) as a wave equation but not a equation for density functions. This is the key point which is distinct from [8] and [9]. As follows, we will show that von Neumann-Landau equation for wave functions Eq.(2.3) is an extension of Schrödinger's wave equation Eq.(2.2) and a suitable form for wave-particle duality.

Since

$$\frac{\partial|\Psi(\vec{x},\vec{y};t)|^2}{\partial t} = 2\text{Re}\left[\Psi^*(\vec{x},\vec{y};t)\frac{\partial\Psi(\vec{x},\vec{y};t)}{\partial t}\right],$$

it is concluded from Eq.(2.3) that

$$\frac{\partial}{\partial t}\int|\Psi(\vec{x},\vec{y};t)|^2\,d^3\vec{x}d^3\vec{y} = 0. \qquad (2.4)$$

This implies that Eq.(2.3) preserves the density $|\Psi(\vec{x},\vec{y};t)|^2\,d^3\vec{x}d^3\vec{y}$ with respect to time and means that, if this wave function Ψ is given at some instant, its behavior at all subsequent instants is determined.

By Schmidt's decomposition theorem [10], for every $\Psi(\vec{x},\vec{y}) \in L^2_{\vec{x},\vec{y}}$ there exist two orthogonal sets $\{\psi_n\}$ and $\{\varphi_n\}$ in $L^2_{\vec{x}}$ and $L^2_{\vec{y}}$ respectively, and a sequence of positive numbers $\{\mu_n\}$ satisfying $\sum_n\mu_n^2 < \infty$ so that

$$\Psi(\vec{x},\vec{y}) = \sum_n\mu_n\psi_n(\vec{x})\varphi_n^*(\vec{y}). \qquad (2.5)$$

Then, it is easy to check that

$$\Psi(\vec{x},\vec{y};t) = \sum_n\mu_n\psi_n(\vec{x},t)\varphi_n^*(\vec{y},t)$$

satisfies Eq.(2.3) with $\Psi(\vec{x},\vec{y};0) = \Psi(\vec{x},\vec{y})$, where both $\psi_n(\vec{x},t)$ and $\varphi_n(\vec{y},t)$ satisfy Eq.(2.2) with $\psi_n(\vec{x},0) = \psi_n(\vec{x})$ and $\varphi_n(\vec{y},0) = \varphi_n(\vec{y})$, respectively. Hence, the wave equation Eq.(2.3) can be solved mathematically from Schrödinger's wave equation.

Also, given $\psi \in L^2_{\vec{x}}$, for every $t \geq 0$ define operators ϱ_t on $L^2_{\vec{x}}$ by

$$(\varrho_t\varphi)(\vec{x}) = \int\Psi(\vec{x},\vec{y};t)\varphi(\vec{y})d^3\vec{y}, \qquad (2.6)$$

where $\Psi(\vec{x},\vec{y};t)$ is the solution of Eq.(2.3) with $\Psi(\vec{x},\vec{y};0) = \psi(\vec{x})\psi^*(\vec{y})$. It is easy to check that

$$i\frac{\partial\varrho_t}{\partial t} = [H,\varrho_t], \quad \varrho_0 = |\psi\rangle\langle\psi|. \qquad (2.7)$$

This is just Schrödinger's equation in the form of density operators. Hence, Schrödinger's wave equation is a special case of the wave equation Eq.(2.3) with initial values of product form $\Psi(\vec{x},\vec{y};0) = \psi(\vec{x})\psi^*(\vec{y})$. This concludes that the wave equation Eq.(2.3) is an extension of Schrödinger's wave equation.

In the sequel, we consider the problem of stationary states. Let ψ_n be the eigenfuncions of the Hamiltonian operator $\hat{H}$, i.e., which satisfy the equation

$$\hat{H}(\vec{x})\psi_n(\vec{x}) = E_n\psi_n(\vec{x}), \qquad (2.8)$$

where E_n are the eigenvalues of $\hat{H}$. Correspondingly, the wave equation Eq.(2.3)

$$i\hbar\frac{\partial\Psi(\vec{x},\vec{y};t)}{\partial t} = \left(\hat{H}(\vec{x}) - \hat{H}(\vec{y})\right)\Psi(\vec{x},\vec{y};t)$$
$$= (E_n - E_m)\Psi(\vec{x},\vec{y};t)$$

with $\Psi(\vec{x},\vec{y};0) = \psi_n(\vec{x})\psi_m^*(\vec{y})$, can be integrated at once with respect to time and gives

$$\Psi(\vec{x},\vec{y};t) = e^{-i\frac{1}{\hbar}(E_n-E_m)t}\psi_n(\vec{x})\psi_m^*(\vec{y}). \qquad (2.9)$$

Since $\{\psi_n(\vec{x})\}$ is a complete orthogonal set in $L^2_{\vec{x}}$, it is concluded that $\{\psi_n(\vec{x})\psi_m^*(\vec{y})\}$ is a complete orthogonal set in $L^2_{\vec{x},\vec{y}}$. Then, for every $\Psi(\vec{x},\vec{y}) \in L^2_{\vec{x},\vec{y}}$ there exists a unique set of numbers $\{c_{n,m}\}$ satisfying $\sum_{n,m}|c_{n,m}|^2 < \infty$ so that

$$\Psi(\vec{x},\vec{y}) = \sum_{n,m}c_{n,m}\psi_n(\vec{x})\psi_m^*(\vec{y}). \qquad (2.10)$$

Hence, for $\Psi(\vec{x},\vec{y};0) = \sum_{n,m}c_{n,m}\psi_n(\vec{x})\psi_m^*(\vec{y})$ we have that

$$\Psi(\vec{x},\vec{y};t) = \sum_{n,m}c_{n,m}e^{-i\frac{1}{\hbar}(E_n-E_m)t}\psi_n(\vec{x})\psi_m^*(\vec{y}) \qquad (2.11)$$

for $t \geq 0$.

Conversely, if $\Psi(\vec{x}, \vec{y}) \in L^2_{\vec{x}, \vec{y}}$ is an eigenfuncion of the operator $\hat{H}(\vec{x}) - \hat{H}(\vec{y})$, i.e., which satisfies the equation

$$\left(\hat{H}(\vec{x}) - \hat{H}(\vec{y})\right)\Psi(\vec{x}, \vec{y}) = \lambda\Psi(\vec{x}, \vec{y}), \qquad (2.12)$$

where λ is an associated eigenvalue, then $\Psi(\vec{x}, \vec{y}; t) = e^{-i\frac{1}{\hbar}\lambda t}\Psi(\vec{x}, \vec{y})$ satisfies Eq.(2.3) and consequently, it is concluded from Eq.(2.11) that $\lambda = E_n - E_m$ is an energy-level gap of the system. Thus, the wave equation Eq.(2.3) can be used to determine energy-level gaps of the system Eq.(2.2).

III.   QUANTUM MEASUREMENT

It is well known that the basis of the mathematical formalism of quantum mechanics lies in the proposition that the state of a system can be described by a definite Schrödinger's wave function of coordinates [5, 8]. As an extension of Schrödinger's wave functions, it seems that the state of a quantum system also can be described by a definite 'bipartite' wave function of Eq.(2.3), of which the physical meaning is that the 'bipartite' wave functions of stationary states determine energy-level gaps of the system.

In fact, we can make the general assumption that if the measurement of an observable $\hat{O}$ for the system in the 'bipartite' state corresponding to Ψ is made a large number of times, the average of all the results obtained will be

$$\langle\hat{O}\rangle_\Psi = \mathrm{Tr}\left[\varrho_\Psi \hat{O} \varrho_\Psi^\dagger\right], \qquad (3.1)$$

where ϱ_Ψ is an operator on L^2 associated with Ψ defined by

$$(\varrho_\Psi \varphi)(\vec{x}) = \int \Psi(\vec{x}, \vec{y})\varphi(\vec{y})d^3\vec{y} \qquad (3.2)$$

for every $\varphi \in L^2$, provided Ψ is normalized since

$$\mathrm{Tr}\varrho_\Psi^\dagger \varrho_\Psi = \int |\Psi(\vec{x}, \vec{y})|^2 d^3\vec{x}d^3\vec{y} = 1. \qquad (3.3)$$

That is, the expectation value of an observable $\hat{O}$ in the 'bipartite' state corresponding to Ψ is determined by Eq.(3.1). In particular, the probability of the system in the 'bipartite' state corresponding to Ψ reduces to a state $|\varphi\rangle$ after measurement is

$$\begin{aligned}
\langle|\varphi\rangle\langle\varphi|\rangle_\Psi &= \mathrm{Tr}\left[\varrho_\Psi|\varphi\rangle\langle\varphi|\varrho_\Psi^\dagger\right] \\
&= \langle\varphi, \varrho_\Psi^\dagger \varrho_\Psi \varphi\rangle \\
&= \|\varrho_\Psi\varphi\|^2 \\
&= \int \left|\int \Psi(\vec{x}, \vec{y})\varphi(\vec{y})d^3\vec{y}\right|^2 d^3\vec{x}.
\end{aligned} \qquad (3.4)$$

It is easy to check that if $\Psi(\vec{x}, \vec{y}) = \psi(\vec{x})\psi^*(\vec{y})$, then $\varrho_\Psi = |\psi\rangle\langle\psi|$ and so

$$\langle\hat{O}\rangle_\Psi = \langle\psi|\hat{O}|\psi\rangle. \qquad (3.5)$$

This concludes that our expression Eq.(3.1) agrees with the interpretation of Schrödinger's wave functions for calculating expectation values of any chosen observable.

IV.   WAVE-PARTICLE DUALITY

Since every normalized 'bipartite' wave function $\Psi(\vec{x}, \vec{y})$ is of the form (2.5) with $\sum_n \mu_n^2 = 1$, we can define the 'entanglement' measure of 'bipartite' wave functions Ψ by

$$S(\Psi) = -\sum_n \mu_n^2 \ln \mu_n^2. \qquad (4.1)$$

It is easy to show that

$$S(\Psi) = -\mathrm{tr}\left[\varrho_{\vec{x}}(\Psi)\ln\varrho_{\vec{x}}(\Psi)\right] = -\mathrm{tr}\left[\varrho_{\vec{y}}(\Psi)\ln\varrho_{\vec{y}}(\Psi)\right], \qquad (4.2)$$

where $\varrho_{\vec{x}}(\Psi) = \mathrm{tr}_{\vec{y}}(|\Psi\rangle\langle\Psi|)$ and $\varrho_{\vec{y}}(\Psi) = \mathrm{tr}_{\vec{x}}(|\Psi\rangle\langle\Psi|)$. Hence, $S(\Psi)$ is the von Neumann's entropy of the reduced density matrix $\varrho_{\vec{x}}(\Psi)$ (or equivalently, $\varrho_{\vec{y}}(\Psi)$) of $|\Psi\rangle\langle\Psi|$ (e.g., [11]). In the sequel, we will show that $S(\Psi)$ is a quantitative measure of complementarity between wave-like and particle-like behaviors.

Let us imagine a screen impermeable to electrons, in which two slits, 1 and 2, are cut. We denote by ψ_1 the wave function of an electron through slit 1 with slit 2 being covered, and ψ_2 the wave function of an electron through slit 2 with slit 1 being covered. Then, the state of a single electron through slits 1 and 2 can be described by a 'bipartite' wave function of form

$$\begin{aligned}
\Psi(\vec{x}, \vec{y}) = {} & a_{11}\psi_1(\vec{x})\psi_1^*(\vec{y}) + a_{12}\psi_1(\vec{x})\psi_2^*(\vec{y}) \\
& + a_{21}\psi_2(\vec{x})\psi_1^*(\vec{y}) + a_{22}\psi_2(\vec{x})\psi_2^*(\vec{y}),
\end{aligned} \qquad (4.3)$$

where $|a_{11}|^2 + |a_{12}|^2 + |a_{21}|^2 + |a_{22}|^2 = 1$. As following are two special cases of (4.3):

$$\Psi_W(\vec{x}, \vec{y}) = \frac{1}{2}\left[\psi_1(\vec{x}) + \psi_2(\vec{x})\right]\left[\psi_1^*(\vec{y}) + \psi_2^*(\vec{y})\right], \quad (4.4)$$

and

$$\Psi_P(\vec{x}, \vec{y}) = \frac{1}{\sqrt{2}}\left[\psi_1(\vec{x})\psi_1^*(\vec{y}) + \psi_2(\vec{x})\psi_2^*(\vec{y})\right]. \qquad (4.5)$$

Accordingly, Ψ_W corresponds to Schrödinger's wave function $\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$, while there is no Schrödinger's wave function associated with Ψ_P. A single electron described by Ψ_W behaves like waves, while by Ψ_P like particles. This is so because for position, by (3.1) we have

$$\langle\hat{x}\rangle_{\Psi_W} = \frac{1}{2}\left|\psi_1(\vec{x}) + \psi_2(\vec{x})\right|^2, \qquad (4.6)$$

and

$$\langle \hat{x} \rangle_{\Psi_P} = \frac{1}{2} \left(|\psi_1(\vec{x})|^2 + |\psi_2(\vec{x})|^2 \right), \qquad (4.7)$$

respectively. Generally, for every Ψ of (4.3) one has

$$0 \leq S(\Psi) \leq S(\Psi_P) = \frac{1}{2} \ln 2.$$

When a single electron is described by Ψ, the larger is $S(\Psi)$, more like particles it behaves. Hence, $S(\Psi)$ characterizes quantitatively wave-particle duality for a single particle. Moreover, $S(\Psi)$ characterizes quantitatively the path entanglement of a single particle in the which-way experiment [12].

V. COLLAPSES OF WAVE FUNCTIONS

Let $\{\psi_n\}$ be the eigenfuncions of the Hamiltonian operator $\hat{H}$. Then, every normalized 'bipartite' wave function $\Psi(\vec{x}, \vec{y})$ can be expressed as (2.10) with $\sum_{n,m} |c_{n,m}|^2 = 1$. Note that

$$\left(\hat{H}(\vec{x}) - \hat{H}(\vec{y}) \right) [\psi_n(\vec{x})\psi_m^*(\vec{y})] = (E_n - E_m) [\psi_n(\vec{x})\psi_m^*(\vec{y})].$$

Then, $c_{n,m}$ can be regarded as the probabilistic amplitude of the transition of the particle from level ψ_n to ψ_m. The probability of getting E_m on measurement in a state with 'bipartite' wave function Ψ is

$$p_m = \sum_n |c_{n,m}|^2. \qquad (5.1)$$

The value of the associated change of energy of the system is

$$\triangle E_m = \sum_n |c_{n,m}|^2 (E_n - E_m). \qquad (5.2)$$

In particular, if $\Psi(\vec{x}, \vec{y}) = \psi(\vec{x})\psi^*(\vec{y})$ with $\psi = \sum_n a_n \psi_n$ and $\sum_n |a_n|^2 = 1$, then $c_{n,m} = a_n a_m^*$ and hence $p_m = |a_m|^2$. In this case, the collapse of ψ to ψ_m can be regarded as the simultaneous transition of the particle from levels $\psi_1, \psi_2, \ldots$ to ψ_m. Thus, our results suggest that von Neumann's collapse of Schrödinger's wave functions is just the simultaneous transition of the particle from many levels to one [8]. We therefore conclude that there are two basic changes for the system of a single particle, one is unitary change, while the other is von Neumann's collapse of wave functions in such a sense that it is the simultaneous transition of the particle from many levels (perhaps, only one) to one.

VI. CONCLUSION

In conclusion, we show that von Neumann-Landau equation for wave functions is an extension of Schrödinger's wave equation and can be used to determine energy-level gaps of the system for a single particle. It is presented a mathematical expression of wave-particle duality and that von Neumann's entropy is a quantitative measure of complementarity between wave-like and particle-like behaviors. Moreover, our formalism suggests that von Neumann's collapse of Schrödinger's wave functions is just the simultaneous transition of the particle from many levels to one.

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